Special Topic : Density operator and matrix (ch. 3.4)

pp 178 – 181

- One of the applications of the Path integral.

① pure vs. mixed state, (or ensemble)

- a pure state : all systems (particles) spins are prepared at $|\Psi\rangle$

↳ Simply, you cannot think of any other possibilities than the system's being at $|\Psi\rangle$

- a mixed state : a set of possible (accessible) states $= \{|\Psi_1\rangle, |\Psi_2\rangle, \cdots\}$.

↳ ex. If you pick up a spin at time t_1, you have $|\Psi_1\rangle$ with some probability. If you pick up another spin at another time, you may have $|\Psi_2\rangle$ with some other probability.

c.f. a linear combination $|\Psi\rangle = c_+|\uparrow\rangle + c_-|\downarrow\rangle$

→ This is a pure state, although it gives you 50% of $|\uparrow\rangle$ or 50% of $|\downarrow\rangle$ in the SG experiment.

- a mixed state : $\{|\uparrow\rangle, |\downarrow\rangle\}$

If you pick one, you may have $|\uparrow\rangle$ with a probability

But, after SG exp. it's 100% of $|\uparrow\rangle$.

Don't be confused.

② The Density operator (matrix)

: a "unified" way to describe a pure and mixed states

- a pure state $\doteq_{\text{def.}}$ $\boxed{\hat{\rho}_{pure} = |\Psi\rangle\langle\Psi|}$.

- a mixed state $\doteq_{\text{def}}$ $\boxed{\hat{\rho}_{mixed} = \sum_i w_i |\Psi_i\rangle\langle\Psi_i|}$

  || w_i : a probability to find $|\Psi_i\rangle$.

- density matrix :

  a matrix representation of $\hat{\rho}$ $\Rightarrow$ $\langle b|\hat{\rho}|a\rangle$

- expectation value of an observable.

$\langle A\rangle = \mathrm{Tr}\,\hat{\rho} A$ ⟶ a pure state

$$\langle A\rangle = \mathrm{Tr}\,|\Psi\rangle\langle\Psi|A = \langle\Psi|A|\Psi\rangle.$$

a mixed state

$$\Rightarrow \langle A\rangle = \sum_i w_i \langle\Psi_i|A|\Psi_i\rangle$$

- Time-evolution.

(ex. pure state)

These are exactly ⇓ the same for $\hat{\rho}_{mixed}$. (HW)

(i) Schrödinger picture.

$$\langle A\rangle_t = \langle\Psi(t)|A|\Psi(t)\rangle = \mathrm{Tr}\,\hat{\rho}(t) A. \qquad \hat{\rho}(t) = U\rho U^{+}$$

(ii) Heisenberg picture || the same !

$$\langle A(t)\rangle = \langle\Psi|A(t)|\Psi\rangle = \mathrm{Tr}\,\hat{\rho}\,A(t)$$

☆ Note : t-evolution of $\hat{\rho}$ $\Rightarrow$ $\boxed{i\hbar\frac{d\hat{\rho}}{dt} = -[\hat{\rho}, H]}$

There's a minus sign!

③ Thermal state (or ensemble)

- Canonical ensemble

$$\hat{\rho} = \frac{e^{-\beta H}}{\mathrm{Tr}\, e^{-\beta H}} \equiv \frac{1}{\underset{\text{"partition function"}}{Z}} \exp[-\beta H] \quad \Big\| \quad \beta = \frac{1}{k_B T}$$

If we know the energy eigenvalues (E_n) and eigenkets $\{|n\rangle\}$,

$$\langle n|\hat{\rho}|m\rangle = \frac{1}{Z} e^{-\beta E_n} \delta_{n,m}$$

: the density matrix is diagonal in the basis of eigenkets.

To see more, attend stat. mech. class!

④ Euclidean Path integral.

: now, time goes into the complex plane.

→ density operator $\hat{\rho} = \frac{1}{Z} e^{-\beta H} = \frac{1}{Z} \mathcal{U}(t=-i\beta\hbar, 0)$

• Path Integral representation of $\mathcal{U}(t,0)$: $\quad \Big\| \; \mathcal{U}(t,0) = e^{-\frac{i}{\hbar}Ht}$

$$\langle x_1|\mathcal{U}(t,0)|x_0\rangle = \int_{\left(\substack{x(0)=x_0 \\ x(t)=x_1}\right)} \mathcal{D}[x(t)] \exp\left[\frac{i}{\hbar} S[x(t)]\right]$$

→ for $\hat{\rho}$,

$$\langle x_1|\mathcal{U}(t=-i\beta\hbar)|x_0\rangle = \int_{\left[\substack{x(0)=x_0 \\ x(t=-i\beta\hbar)=x_1}\right.} \mathcal{D}[x(t)] \exp\left[\frac{i}{\hbar} S\right]$$

• Action at $it = t_E$. (Euclidean, ~~complex~~ imaginary time)

$$\frac{iS}{\hbar} = \frac{i}{\hbar} \int_0^{-i\beta\hbar} dt\, L(x, \dot{x})$$

$$= -\frac{1}{\hbar} \int_0^{\beta\hbar} dt_E \left[-L\left(x, i\frac{dx}{dt_E}\right)\right] = -\frac{1}{\hbar} \boxed{\int_0^{\beta\hbar} dt_E \underbrace{\left[\frac{1}{2}m\left(\frac{dx}{dt_E}\right)^2 + V\right]}_{=H}} = \text{Euclidean Action "}S_E\text{"}$$

$$\Rightarrow \hat{\rho} = Z^{-1} \int_{0 \to \beta\hbar} \mathcal{D}[x(\tau_E)] \exp\left[-\frac{1}{\hbar} S_E[x(\tau_E)] \right] \quad \begin{cases} x(0) = x_0 \\ x(\beta\hbar) = x_1 \end{cases}$$

No complex number!

and

$$Z = \mathrm{Tr}\, e^{-\beta H} = \int dx \langle x | U(t=-i\beta\hbar, 0) | x \rangle$$

$$= \int dx\, K(x, -i\beta\hbar; x, 0) = \int_{x(0)=x(\beta\hbar)} \mathcal{D}[x(\tau_E)] \exp\left[-\frac{1}{\hbar} S_E \right]$$

ex 1. a simple harmonic oscillator

$$K(x,t;x_0,t_0) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin[\omega(t-t_0)]}} \exp\left[\left(\frac{i m\omega}{2\hbar \sin[\omega(t-t_0)]} \right) \cdot \left[(x^2+x_0^2)\cos[\omega(t-t_0)] - 2xx_0 \right] \right]$$

... (2.6.18) Sakurai

↓ partition fn.

$$Z = \int_{-\infty}^{\infty} dx\, K(x, -i\beta\hbar; x, 0) = \int_{-\infty}^{\infty} dx \sqrt{\frac{m\omega}{2\pi\hbar \sinh(\beta\hbar\omega)}} \exp\left[- \frac{x^2}{\left[\frac{\hbar \sinh(\beta\hbar\omega)}{m\omega(\cosh(\beta\hbar\omega)-1)} \right]} \right]$$

$$= \frac{1}{\sqrt{2(\cosh(\beta\hbar\omega)-1)}} = \frac{e^{-\beta\hbar\omega/2}}{1-e^{-\beta\hbar\omega}} = \sum_{n=0}^{\infty} e^{-\beta E_n}$$

!!!

ex 2. Expectation values of $A(x)$

$$\langle A(\hat{x}) \rangle = \mathrm{Tr}\, \rho A = Z^{-1} \int dx\, A(x) \langle x | e^{-\beta H} | x \rangle$$

$$= \frac{\int dx_0 \int_{x(0)=x(\beta\hbar)=x_0} \mathcal{D}[x(\tau)]\, A(x_0) \exp\left[-\frac{1}{\hbar} S_E[x(\tau)] \right]}{\int_{x(0)=x(\beta\hbar)} \mathcal{D}[x(\tau)] \exp\left[-\frac{1}{\hbar} S_E \right]}$$

ex 3.

2-point correlation function $\langle x(t)\, x(0) \rangle_\beta$

"Kubo-Martin-Schwinger (KMS) condition"

$$\langle x(t)\, x(0) \rangle_\beta = \mathrm{Tr}\left[x(t)\, x(0)\, U(-i\beta\hbar) \right] = \mathrm{Tr}\left[e^{\frac{i}{\hbar}Ht} x\, e^{-\frac{i}{\hbar}Ht} x\, e^{-\beta H} \right]$$

$$= \mathrm{Tr}\left[e^{\frac{i}{\hbar}H(t+i\beta\hbar)} x\, e^{-\frac{i}{\hbar}H(t+i\beta\hbar)} e^{-\beta H} \cdot x \right]$$

$$= \langle x(0)\, x(t+i\beta\hbar) \rangle_\beta$$: "periodicity in complex-t"

2-7 Gauge transformations

– Gauge invariance in the classical electrodynamics

$$\vec{E}(\vec{x},t) = -\nabla\phi(\vec{x},t) - \frac{1}{c}\frac{\partial}{\partial t}\vec{A}(\vec{x},t)$$
$$\vec{B}(\vec{x},t) = \nabla\times\vec{A}(\vec{x},t)$$

[CGS unit]

$\vec{E}$ and $\vec{B}$ are invariant under the "gauge" transformation.

$$\Rightarrow \quad \vec{A}(\vec{x},t) \rightarrow \vec{A}(\vec{x},t) + \nabla\Lambda(\vec{x},t)$$
$$\phi(\vec{x},t) \rightarrow \phi(\vec{x},t) - \frac{1}{c}\frac{\partial}{\partial t}\Lambda(\vec{x},t)$$

But it introduces a phase factor in the quantum state!

$$\Rightarrow \quad |\alpha,t\rangle \rightarrow \exp\left[\frac{ie}{\hbar c}\Lambda\right]|\alpha,t\rangle$$

✻ In QM, this is not just about EM-fields but quite general.

① A simple example : Constant potentials

→ $V(\vec{x}) \rightarrow V(\vec{x}) + V_0$ (a constant shift)

: It does not change a thing in the classical Mechanics.

But, let's look at the time evolution of $|\alpha\rangle$.

i) $H = T + V$: $|\alpha,t\rangle = \exp\left[-\frac{i}{\hbar}(T+V)t\right]|\alpha\rangle$

ii) $H = T+V+V_0$: $|\alpha,t\rangle = \exp\left[-\frac{i}{\hbar}(T+V+V_0)t\right]|\alpha\rangle$

Thus, $|\alpha,t\rangle \longrightarrow \exp\left[-\frac{i}{\hbar}V_0 t\right]|\alpha,t\rangle$

as $V(\vec{x}) \rightarrow V(\vec{x}) + V_0$.

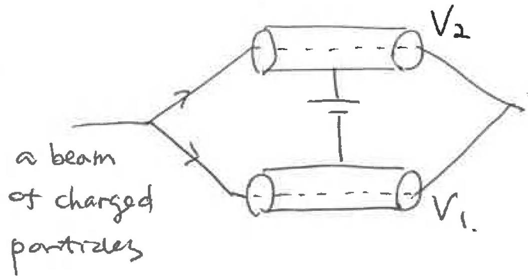
If $V_0 \equiv V_0(t)$,

$$|\alpha, t\rangle \longrightarrow \exp\left[-\frac{i}{\hbar}\int_0^t dt' \, V_0(t')\right] |\alpha, t\rangle$$

* This phase factor is "purely" quantum-mechanical!

and it can appear in measurements.
(interferometers).

ex.



Interference.

due to the phase diff.

$$\phi_1 - \phi_2 = \frac{1}{\hbar}(V_2 - V_1)\underbrace{\Delta t}_{\text{travel time}}.$$

ex. Gravity in QM.

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + m\Phi_{grav}\right]\psi = i\hbar\frac{\partial\psi}{\partial t}.$$

$\longrightarrow$ Φ_{grav} is too small to cause any measurable changes

in the observables.

ex. electron - neutron binding due to gravity $\to \frac{G m_e m_n}{r^2}$

vs.

electro - proton binding due to Coulomb forces. $\to \frac{e^2}{r^2}$

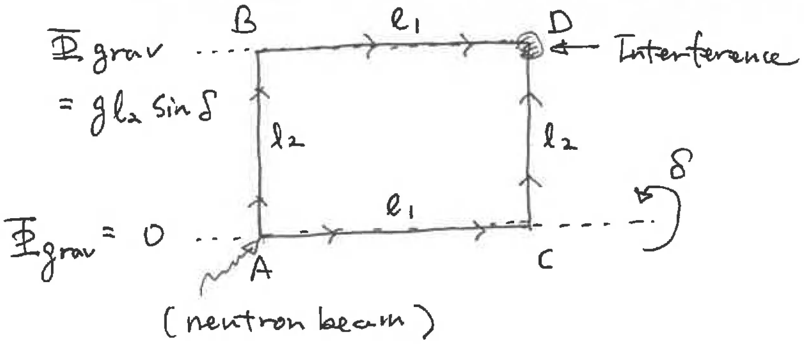
$\hookrightarrow$ $a_0 = \frac{\hbar^2}{e^2 m_e}$ (Bohr radius).

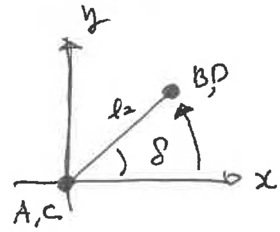
$\downarrow$

$$\frac{\hbar^2}{G m_e^2 m_n} \sim 10^{31} \text{ light years!}.$$

But it introduces the phase factor to $|\psi\rangle$

$\longrightarrow$ gravity-induced quantum interference.





$$\Rightarrow \text{phase factor} = \exp\left[-\frac{i}{\hbar} m_n g l_2 \sin\delta \cdot \underset{\uparrow}{T}\right]$$

Travel time along $\overline{BD}$

$$T = \frac{l_1}{v_n} \simeq l_1 \Big/ \frac{\hbar}{m\lambda\!\!\!^{-}}$$

$\lambda\!\!\!^{-}$: de Broglie wavelength $= \dfrac{\hbar}{p} = \dfrac{\hbar}{m v_n}$

② Back to the EM fields : a charged particle in the EM-fields.

- Review on the classical mechanics.

a charge (if it's electron, $e<0$)

i) Lagrangian : $$L = \frac{1}{2} m \dot{\vec{x}}^2 - e\phi + \frac{e}{c}\, \dot{\vec{x}} \cdot \vec{A}(\vec{x},t)$$

EOM : $$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}_i}\right) - \frac{\partial L}{\partial x_i} = 0$$

$$\frac{\partial L}{\partial \dot{x}_i} = m\dot{x}_i + \frac{e}{c} A_i, \qquad \frac{\partial L}{\partial x_i} = -e\frac{\partial \phi}{\partial x_i} + \sum_j \frac{e}{c}\dot{x}_j \frac{\partial A_j}{\partial x_i}$$

$$\Rightarrow \quad m\ddot{x}_i + \frac{e}{c}\left(\frac{\partial A_i}{\partial t} + \sum_j \frac{\partial A_i}{\partial x_j}\dot{x}_j\right) + e\frac{\partial \phi}{\partial x_i} - \sum_j \frac{e}{c}\dot{x}_j \frac{\partial A_j}{\partial x_i} = 0.$$

$$m\ddot{x}_i = -e\left[\frac{\partial \phi}{\partial x_i} + \frac{1}{c}\frac{\partial A_i}{\partial t}\right] + \frac{e}{c}\sum_j\left[\dot{x}_j \frac{\partial A_j}{\partial x_i} - \dot{x}_j \frac{\partial A_i}{\partial x_j}\right]$$

$$\left[\frac{\partial \phi}{\partial x_i} + \frac{1}{c}\frac{\partial A_i}{\partial t}\right] = \Big(\nabla\phi + \frac{1}{c}\frac{\partial \vec{A}}{\partial t}\Big)_i = (-\vec{E})_i$$

$$\sum_j\left[\dot{x}_j \frac{\partial A_j}{\partial x_i} - \dot{x}_j \frac{\partial A_i}{\partial x_j}\right] = \dot{x}_j\, \varepsilon_{ijk}\, \underbrace{(\nabla\times\vec{A})_k}_{=\vec{B}} = (\dot{\vec{x}}\times\vec{B})_i$$

$$\Rightarrow \quad m\ddot{\vec{x}} = e\vec{E} + \frac{e}{c}\,\dot{\vec{x}}\times\vec{B}$$

The Lagrangian is verified.